University of California
Lawrence Livermore
National Laboratory

ASCI Three-Dimensional Hydrodynamic Instability and Turbulence Modeling

Objective

We are studying turbulence processes in strongly-compressible three-dimensional hydrodynamic flows and developing subgrid-scale parameterizations of turbulence effects for large-eddy numerical simulations.

Impact

Three-dimensional, compressible fluid turbulence simulations are necessary for carrying out computations that are essential to maintaining the safety, reliability, and performance of the U.S. nuclear stockpile.

In many hydrodynamics applications, the relevant length scales range over several orders of magnitude, so that finite-difference direct numerical simulations (DNS) are computationally not feasible for the driving parameters of interest. To simulate the dynamically important range of scales, we perform large-eddy simulations (LES) instead, in which the dynamical effects of the unresolved scales are modeled by a subgrid-scale parameterization, and the resolved scales are calculated explicitly. These parameterizations allow the use of fewer gridpoints than would be necessary for a DNS. Thus, a principal research topic in this project is to develop subgrid-scale parameterizations from hydrodynamic theory and experiments and to validate them against fully resolved DNS and available experimental data.

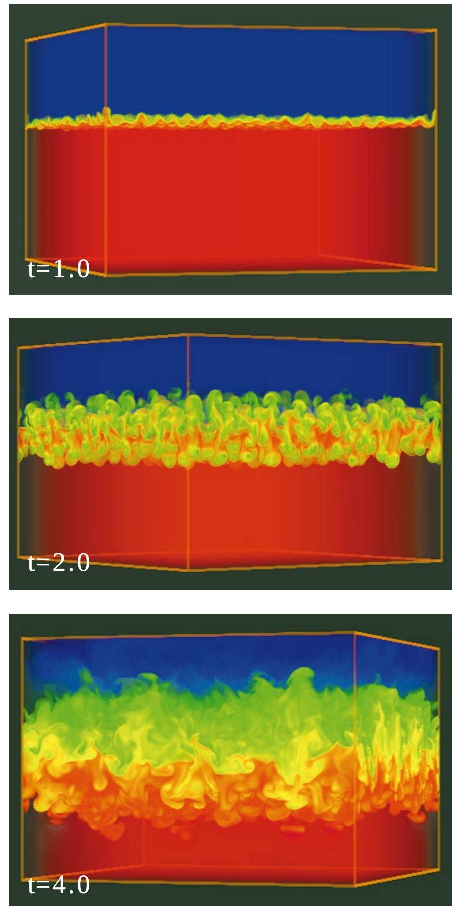
Three-Dimensional Compressible Turbulence Simulations

A major thrust of the ASCI applications programs is a shift from two-dimensional to three-dimensional physics computations. Turbulence in two and three dimensions is profoundly different. For example, in a two-dimensional flow, small-scale fluctuations can often coalesce into larger-scale structures, so that energy is transferred from small scales to larger scales. In three dimensions, large-scale structures tend to break up into smaller structures, with a transfer of energy from the large scales to smaller scales. This has important consequences for both simulations and physics.

In two-dimensional simulations of two-dimensional physics, fluctuations on resolved scales can often be accurately captured as long as there is some dissipation at the smallest scales. However, in two-dimensional simulations of three-dimensional physics, the average effects of three-dimensionality are calculated separately and incorporated as a transport process in two-dimensional space.

In three-dimensional DNS, three-dimensional turbulence can be directly simulated, but only over a limited range of length scales. Even if the initial fluctuations are restricted to resolved scales, the turbulence dynamics can induce transfer of energy to length scales that are too small to resolve. It is thus essential for physics reasons, and can also be important for numerical reasons, to incorporate a subgrid-scale parameterization that adequately approximates the effect of these smaller unresolved length scales on the larger resolved scales.

Another important consequence of the difference between two- and three-dimensional turbulence dynamics is that parameterizations developed to characterize two-dimensional turbulence are likely to be inadequate for three-dimensional turbulence. Furthermore, when studying three-dimensional turbulence, the parameterizations that are accurate for LES will in general differ from those that are accurate for two-dimensional transport modeling, because they must represent the effects of a different degree of averaging in the third direction.



This figure shows the mixing of the heavier fluid, which is initially on top, with the fluid on the bottom. This is known as the Rayleigh-Taylor instability.

Numerical Approach

We are using a numerical simulation code based on the piecewise parabolic method (PPM), which is a higher-order accurate Godunov method developed by Colella and Woodward. The Godunov approach is typical of standard numerical techniques in regions where the solution

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is smooth. However, in regions with discontinuities, such as strong shocks, the Godunov method approximates the solution well by analytically solving an associated Riemann problem. This is an idealized problem describing the evolution of a simple jump into shocks and/or rarefactions, with a contact discontinuity in between. Monotonicity constraints ensure that these discontinuities remain sharp and accurate as they traverse the computational grid. The higher-order spatial interpolation in the PPM allows steeper representation of discontinuities, thus allowing a more accurate solution to a wider class of problems. For some of our simulations, molecular dissipation processes are explicitly modeled, in which case the simulations are of the Navier-Stokes equations rather than the Euler equations.

Programming Model

We are using the PPM code of Woodward and coworkers, in which parallelization is implemented by domain decomposition with message-passing. The subdomains are three-dimensional and contain extra border cells to allow intermediate computation, to reduce the required interprocessor communication. The border communications are decomposed into one-dimensional shifts and are easily adaptable to new architectures. Variables are ordered in memory to effect optimal usage of cache. To date, we have run calculations on the IBM-SP at LLNL, the LLNL DEC Alpha machine (using a single processor), the LLNL T3D, the Sandia Paragon, the Sandia Red Machine prototype, and the IBM-SP at the Cornell Theory Center.

Application Areas

We are presently studying two general categories of compressible turbulent processes: (1) homogeneous, isotropic turbulence subject to a variety of forcing mechanisms including the passage of shocks, and (2) the development and evolution of turbulence in a strongly stratified medium subjected to continuous (Rayleigh-Taylor) or impulsive (Richtmyer-Meshkov) acceleration. For the former, benchmark datasets resulting from DNS are used to validate statistical two-point closures (models involving correlations between two points in space for closing the fluid equations) at computationally affordable driving levels, and transport scaling properties are extracted from the validated closures at the high driving levels representative of the applications. This, together with appropriate analytical limits of the closure equations, leads to subgrid-scale parameterizations.

We are collaborating with Paul Woodward and David Porter of the University of Minnesota, both in this regard and with respect to use of their PPM code in general. In the latter area, we are collaborating with Steven Orszag of Cambridge Hydrodynamics Inc. to develop a hybrid model based on a direct simulation of the largest “bubbles” and “spikes” that arise when fluids mix, a bubble merger model to describe unresolved bubbles and spikes, and a model to describe the turbulence resulting from secondary Kelvin-Helmholtz instabilities.

Rayleigh-Taylor Instability and Turbulent Mixing

As an example of our research, we use the PPM code to simulate the Rayleigh-Taylor instability and turbulent mixing on a unit cube spanned by a grid containing 512 points in each of the three directions. This case was run on the ASCI Blue-Pacific ID System at LLNL using 128 nodes. The initial equilibrium state consists of a gamma = 5/3 gas, in which the subvolumes above and below the midplane (z = 0.5) are stably stratified equilibria. The internal energies are piecewise constant, while the density and pressure decrease exponentially with height, but have different scale heights above and below the midplane. The density has a jump from 1 just below, to 2 just above the midplane, corresponding to an Atwood number of 1/3, and the pressure is continuous across the midplane. The sound speed corresponding to the equilibrium state below the midplane is 1.0. Other parameters are Prandtl number = 1.0 and viscosity = 0.00004. The boundaries are periodic in the horizontal directions and impenetrable in the vertical direction.

A random spectrum of low-level velocity perturbations away from the equilibrium state is initially imposed. The figure (on the front side) shows the temperature field at times t = 1.0, 2.0, and 4.0. After the initial linear mixing phase, bubbles (rising from below) and spikes (falling from above) begin to form. Afterward, the horizontal fluctuation scales grow in size and the physical system evolves toward a stably stratified equilibrium.

Evaluation of High-Performance Computing Platforms

This project has an important secondary goal, that of exploring the limits of ASCI high-performance computing platforms for three-dimensional hydrodynamics applications. This would include scalable, distributed memory massively parallel processors as well as shared memory processor (SMP) clusters. Our high demands on data storage, visualization, and archival storage will test the robustness of the problem-solving environment as well.

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